

## Crystal structure and interaction of 6-amino coumarin with nitrite ion for its selective fluorescence detection

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### Abstract

6-Amino coumarin has been established as an efficient nitrite ion selective fluorescent sensor. The developed method shows linearity up to  $1.6 \times 10^{-6}$  molL<sup>-1</sup> of nitrite ion concentration. Interference from other common anions is almost negligible. The reagent shows strong binding affinity towards nitrite ion as evident from its binding constant value ( $5.8 \times 10^4$ ), estimated by Stern-Volmer method. Some real samples were analyzed. Single crystal X-ray structure of the reagent is reported. Preliminary computational studies on the molecular level interaction between the reagent and nitrite ion were performed by density functional theory (DFT, B3LYP) method. Copyright © 2012 Taylor and Francis Group, LLC.

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### Keywords

6-amino coumarin, computational studies, crystal structure, fluorescence, nitrite